

Ecotox Report for Case # P-16-0400

General

Status: 11/21/2018
Date:
SAT Date: 06/17/2016
Consolidated PMN: N
Ecotox: [REDACTED]
Related Cases: [REDACTED]
Health Related Cases: [REDACTED]
Submitter: Shell Chemical LP
CAS Number: 1809170-78-2
Chemical Name: Alkanes, C11-16-branched and linear
Use: Solvent/diluent in coatings (25%), cleaning fluids (9.5%), agrochemicals (3.2%), and metalworking fluids/rolling oils (8.9%), and as a chemical intermediate (53.4%). [REDACTED]
Trade Name: GTL Solvent GS1927, GS9127
PV-max(kg/yr): 63500000.0000
Report Status: Complete
CRSS Date: 06/16/2016
SAT Chair: Becky Daiss
Consolidated Set:

Fate Summary Statement

Fate P-16-0400

Summary

Statement: FATE: Estimations for low weight n-undecane, C₁₁H₂₄, MW 156.31

Liquid with MP = -26 °C (M)

log Kow = 5.74 (E)

S = 0.004 mg/L

at 25 °C (M)

VP = 0.412 torr at 25 °C (M)

BP = 196 °C (M)

H =
 1.93 (E)
 log Koc = 3.42 (E)
 log Fish BCF = 2.08 (E)
 log Fish
 BAF = 3.30 (E)
 POTW removal (%) = 90 via sorption, stripping and
 biodeg
 Time for complete ultimate aerobic biodeg = wk-mo
 Sorption
 to soils/sediments = moderate-strong
 Volatilization half-life from a
 standard river = 1 hrs
 Volatilization half-life from a standard lake =
 5 da
 Atmospheric Oxidation Half-life = 10 hr via OH radical
 PBT
 Potential: P1-2B1-2
 *CEB FATE: Migration to ground water =
 slow-moderate

Physical Chemical Information

Molecular Weight:	156.31	
Wt% < 500:		Wt% < 1000:
Physical State - Neat:	Liquid	
Melting Point:		Melting Point (est):
MP (EPI):	-25.60	
Vapor Pressure:		Vapor Pressure (est):
VP (EPI):	4.12e-001	
Water Solubility:		Water Solubility (est):
Water Solubility (EPI):		0.000004
Henry's Law::		
Log Koc:		Log Koc (EPI):
Log Kow:		Log Kow (EPI):
		5.74

<p align="center">Log</p> <p>Kow Comment:</p>

SAT
Concern Level

<p>Ecotox 3</p> <p>Rating (1):</p> <p>Ecotox chronic</p> <p>Rating Comment concerns only</p> <p>(1):</p> <p>Ecotox Rating</p> <p>(2):</p> <p>Ecotox Rating</p> <p>Comment (2):</p> <p>Ecotox All</p> <p>Route of releases to water</p> <p>Exposure:</p>

Ecotox
Comments

<p>Exposure Based Y</p> <p>Review (Eco):</p> <p>Ecotox</p> <p>Comments:</p> <p>Exposure Based</p> <p>Testing:</p>

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1-2	1-2	2	1st rating for linear components, 2nd rating for branched components

Eco-Toxicity Comment:

Fate Ratings

<p>Removal90</p> <p>in WWT/POTW</p> <p>(Overall):</p> <p>Condition</p> <p>Rating</p> <p>Values</p> <p>1</p> <p>2</p> <p>3</p> <p>4</p> <p>Rating Description</p> <p>Comment</p> <p>Fish BCF:</p>

Removal ⁹⁰ in WWT/POTW (Overall): Condition						
Rating Values	1	2	Rating Description		4	Comment
			3			
Log Fish BCF:						
WWT/POTW Sorption:	2-3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	2-4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2-4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2-3	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	2-3	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	2-3	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:						
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	*		See the revised hazard under document uploaded 1-5-2018 and see attached supporting documents.
Daphnid	48-h	LC50	*		"
Green Algae	96-h	EC50	*		"
Fish	-	Chronic Value	0.008		"
Daphnid	-	Chronic Value	0.011		"
Green Algae	-	Chronic Value	*		"
Ecotox Value Predictions are based on SARs for neutral organic chemicals; SAR chemical class = hydrocarbon; MW 419; liquid with mp unknown (P); S = 0.004 mg/L at 20 C (P); pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;					

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):		5/10		*; See the revised hazard under document uploaded 1-5-2018 and see attached supporting documents.
Chronic Aquatic(ppb):			1	See the revised hazard under document uploaded 1-5-2018 and see attached supporting documents.
Factors	Values	Comments		
SARs:	neutral organic chemicals			
SAR	hydrocarbon			
Class:				
TSCA NCC				
Category?	Neutral Organics			

Recommended

Testing:

Ecotox Factors See

Comments: Post-Focus Revised Environmental Hazard and Risk Language for P-16-0400 dated 11-19-2018.

See attachments "Revised Ecotoxicity Assessment for P-16-0400 1-5-2018" and supporting documents [REDACTED] and "Final Amended Review of Ecotox Studies for [REDACTED] for revised hazard and risk assessment.

November 19, 2018

Post-Focus Revised
Environmental Hazard and Risk Language for P-16-0400

Environmental

Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated acute hazard for the low molecular weight species (MW 156.21; n-undecane, [REDACTED] for this PMN substance using the Ecological

Structure Activity Relationships (ECOSAR) Predictive Model (<https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>); specifically, the QSAR for the class of neutral organics. EPA estimated chronic environmental hazard of this new chemical substance using data on analogous chemicals [REDACTED] This substance falls within the TSCA New Chemicals Category Neutral Organics. The acute and chronic toxicity values for fish, daphnia, and algae are estimated to be no effects at saturation. The toxicity values for both the new chemical substance and the low molecular weight species indicate the PMN substance is expected to have low hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Environmental Risk: Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environment from acute and chronic exposure are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at

saturation).

Ecotox Assessor: T.
Wright

Comments/Telephone Log

Artifact	Update/Upload Time
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